Exact first-passage exponents of 1D domain growth: relation to a reaction-diffusion model

Bernard Derrida[†‡], Vincent Hakim[†] and Vincent Pasquier[‡]
† *Laboratoire de Physique Statistique, 24 rue Lhomond, 75231 Paris Cedex 05, France.*
‡*Service de Physique Théorique CE Saclay,F91191 Gif sur Yvette, France.*

In the zero temperature Glauber dynamics of the ferromagnetic Ising or q-state Potts model, the size of domains is known to grow like $t^{1/2}$. Recent simulations have shown that the fraction $r(q,t)$ of spins which have never flipped up to time t decays like a power law $r(q,t) \sim t^{-\theta(q)}$ with a non-trivial dependence of the exponent $\theta(q)$ on q and on space dimension. By mapping the problem on an exactly soluble one-species coagulation model ($A + A \to A$), we obtain the exact expression of $\theta(q)$ in dimension one.

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Phase ordering and domain growth in systems quenched from a disordered phase to an ordered phase has been a subject of much interest during the last fifteen years in fields ranging from metallurgy to cosmology [1]. It is well established that the pattern of growing domains is self-similar in time and that the characteristic domain size increases with a simple power law t^{ρ}. For example, $\rho = 1/2$ holds for all systems with short range-interactions described by a scalar non-conserved order parameter. However, as noted for the auto-correlation function [2], correlations at different times are characterized by more complicated exponents. Recently, the fraction of spins $r(q,t)$ which have never flipped up to time t has been measured in simulations of coarsening at zero-temperature for the Ising and for the q-state Potts models. This fraction decreases with time like a power law [3,4],

$$r(q,t) \sim t^{-\theta(q)} \tag{1}$$

and numerical data indicate that the exponent $\theta(q)$ varies both with q and the dimension of space. Since $dr(q,t)/dt$ measures the probability that a given point is crossed for the first time at time t by a domain wall, $\theta(q)$ can be viewed as a first passage exponent [5].

The aim of the present letter is to give the exact expression of $\theta(q)$ in one dimension.

$$\theta(q) = -\frac{1}{8} + \frac{2}{\pi^2}\left[\cos^{-1}\left(\frac{2-q}{\sqrt{2}\,q}\right)\right]^2 \tag{2}$$

This result fully agrees with previous numerical predictions based on MonteCarlo simulations [3,4] or on finite size scaling calculations [6]. It implies that for the Ising model $\theta(2) = 3/8$ is exact. Note however that for other choices of q, the exponent $\theta(q)$ is in general irrational (for example $\theta(3) = .53795082..$).

To obtain (2), we are going to follow four main steps: first by using finite size scaling we will relate the exponent $\theta(q)$ to the large L behavior of the fraction $\rho_L(q)$ of spins which never flip between time 0 and time ∞ for a finite one dimensional system of L sites with periodic boundary conditions (for the zero temperature Glauber dynamics of the q-state Potts model); secondly, we will show that the calculation of $\rho_L(q)$ can be reduced to solving the steady state of a reaction-diffusion model ($A + A \to A$) on a one dimensional lattice of L sites with a source of particles at the origin (i.e. at site $0 \equiv L$); our third step will be the solution of the steady state of that reaction-diffusion model leading to the exact expression of $\rho_L(q)$ for arbitrary L and q; lastly, we will extract the exponent $\theta(q)$ from the large L behavior of this expression.

In an infinite system, it is known [7,8] that starting with a random initial condition, the size of domains grows like $t^{1/2}$. For a finite system of size L, one expects the dynamics to be very much the same as for the infinite system when $t \ll L^2$ (as the size of domains is small compared to the system size). On the other hand, for $t \gg L^2$, there is a single domain left in the system and the dynamics stops. Therefore one expects that $\rho_L(q) \sim r(q, L^2)$ which implies that

$$\rho_L(q) \sim L^{-2\theta(q)} \tag{3}$$

We obtain, in what follows, an exact expression of $\rho_L(q)$ valid for all sizes L and (3) will allow us to extract then the exponent $\theta(q)$.

We now show that the calculation of $\rho_L(q)$ is equivalent to solving the following reaction-diffusion [9] model ($A+A \to A$) defined on a ring of L sites with a source of particles at the origin (that we choose to be at site $L \equiv 0$): the origin

(site L) is always occupied and the other sites i (for $1 \leq i \leq L-1$) are either occupied by a particle A or empty; during every infinitesimal time interval dt, each particle hops with probability dt to its right neighbor and with probability dt to its left neighbor (and does not move with probability $1-2dt$); if two particles occupy the same site, they instantaneously coagulate ($A+A \to A$); in addition whenever the particle at the origin jumps to one of its neighbors, a new particle is instantaneously produced at the origin.

In the steady state, injection of particles at the origin is balanced by aggregation of particles in the bulk and one has a probability $P_L(m)$ of finding m sites occupied on the ring of L sites. The connection with the spin problem described above is made [6] by expressing the probability $\rho_L(q)$ of never flipping (from $t=0$ until $t=\infty$) in terms of $P_L(m)$

$$\rho_L(q) = \sum_{m=1}^{L} P_L(m) \frac{1}{q^{m-1}} \quad . \tag{4}$$

This formula is obtained by remembering that updating a spin in one dimension with Glauber dynamics at zero temperature simply consists in choosing for its new value the value of one of its two neighbors at random. When the value V of a spin S_i at time t is traced back in time, a random walk is obtained which connects $S_i(t)$ through various ancestors to a particular spin in the initial configuration with value V. Now, let us consider all the updates of the spin at the origin. They all give rise to random walks going backward in time. These walks can merge and are created at the origin exactly as in the one species coagulation model. So, in the limit $t \to \infty$, they lead to m different ancestors in the initial configuration with probability $P_L(m)$. Equation (4) then follows by noting that the spins in the initial configuration are uncorrelated and that the spin at the origin never flips if and only if all its updates have the same value.

We now come to the full exact solution of the reaction-diffusion model steady state which is the crucial point of the present work. It is known that some properties of the coagulation model $A+A \to A$ can be calculated exactly [10] even in the presence of a fixed source [11]. The properties which have been calculated [10] so far on this sort of problems are the probabilities that a (connected) region of consecutive sites are all empty. This is because one can obtain closed kinetic equations (see (5) below) for these quantities. The key to our exact solution is that more complicated quantities like the probability of having 2 (or 3 or $\cdots n$) disconnected empty regions can be expressed in a simple way in terms of these probabilities that a single connected region is empty.

Let us define for the coagulation model the probabilities $B_{i,j},\ 1 \leq i < j \leq L$ that the segment $\{i, i+1, ..., j-1\}$ contains no particle [10,6]. These quantities change when a particle enters or leaves the segment through its extremities and this can be expressed in terms of the $B_{i,j}$ themselves (for example, the probability to find a particle at site j given that sites $i, i+1, \cdots, j-1$ are empty is $B_{i,j} - B_{i,j+1}$). Therefore, the $B_{i,j}$'s satisfy closed kinetic equations which read in the steady state

$$B_{i+1,j} + B_{i-1,j} + B_{i,j+1} + B_{i,j-1} - 4B_{i,j} = 0 \tag{5}$$

Modified equations for $j = i+1$ and boundary conditions coming from the permanent occupation of the origin can be taken into account by the conventions $B_{i,i} = 1$ and $B_{0,j} = B_{i,L+1} = 0$.

The explicit solution of (5) is [6]:

$$B_{i,j} = \sum_{k\ even} \sum_{k'\ odd} \frac{8 \sin k\alpha\ \sin k'\alpha\ (\sin ki\alpha\ \sin k'j\alpha\ -\ \sin kj\alpha\ \sin k'i\alpha)}{(L+1)^2\ (\cos k'\alpha\ -\ \cos k\alpha)\ (2 - \cos k\alpha - \cos k'\alpha)}\ ,\quad i<j \tag{6}$$

with $\alpha = \pi/(L+1),\ 2 \leq k \leq L,\ 1 \leq k' \leq L$ (Note that (6) is not valid for $j=i$ since it gives $B_{ii}=0$ instead of 1). For example, when $L=4$, this gives $B_{1,2} = B_{3,4} = 26/44; B_{1,3} = B_{2,4} = 16/44; B_{1,4} = 8/44; B_{2,3} = 30/44$.

These known results can be generalized by introducing the probabilities $B^{(n)}_{i_1,i_2,\cdots,i_{2n-1},i_{2n}}$ that there is no particle in any of the disconnected segments $\{i_1, i_1+1, \cdots, i_2-1\}, \cdots \{i_{2n-1}, \cdots, i_{2n}-1\}$ with $i_1 < i_2 < \cdots < i_{2n}$. Similarly to the $B_{i,j}$'s (to which they reduce for $n=1$), the $B^{(n)}$'s satisfy equations analogous to (5). The new boundary conditions can be taken care of by the convention that $B^{(n)}$ reduces to the corresponding $B^{(n-1)}$ if two successive indices coincide.

It turns out that the diffusion-like equations satisfied by the $B^{(n)}$'s can be solved exactly and that their solutions can all be expressed in terms of the $B_{i,j}$. Namely,

$$B^{(2)}_{i,j,k,l} = B_{i,j}B_{k,l} + B_{i,l}B_{j,k} - B_{i,k}B_{j,l} \tag{7}$$

and more generally

$$B^{(n)}_{i_1,i_2,\ldots,i_{2n-1},i_{2n}} = \frac{1}{2^n\ n!} \sum_\sigma \epsilon(\sigma) B_{i_{\sigma(1)},i_{\sigma(2)}} \cdots B_{i_{\sigma(2n-1)},i_{\sigma(2n)}} \tag{8}$$

where the sum runs over all the permutations of the indices $\{i_1, i_2, \cdots, i_{2n}\}$ and $\epsilon(\sigma)$ is the signature of the permutation σ (Note that (7) and (8) are Pfaffians [12]). One way to prove (7-8) is simply to check that their r.h.s. satisfy the same diffusion-like equations as the $B^{(n)}$'s when $B_{i,j}$ is solution of (5) and that they indeed reduce to the expression for $B^{(n-1)}$ if two successive indices coincide. In the case $L = 4$, one finds that $B^{(2)}_{1,2,3,4} = 15/44$.

Once the $B^{(n)}$'s are known, all the steady state properties of the reaction-diffusion model are in principle computable, in particular the $P_L(m)$, and as a consequence (4) the $\rho_L(q)$. There is a simple way of obtaining the $\rho_L(q)$ in terms of the $B^{(n)}$'s: introduce the (normalized) weights $w(\tau_1, \cdots \tau_{L-1})$ in the steady state of configuration $\{\tau_1, \cdots \tau_{L-1}\}$ (where $\tau_i = 1$ if site i is occupied and $\tau_i = 0$ if it is emtpy); we can write the sum over possible particle numbers in the steady state in eq.(4) as an explicit sum over all possible configurations

$$\sum_{m=1}^{L} P_L(m)\ \frac{1}{q^{m-1}} = \sum_{\tau_1,\cdots\tau_{L-1}} \frac{w(\tau_1, \cdots, \tau_{L-1})}{q^{\tau_1+\cdots+\tau_{L-1}}} \tag{9}$$

Using the identity $q^{1-\tau_1+\ldots+1-\tau_{L-1}} = \prod_{j=1}^{L-1}[1 + (q-1)(1-\tau_j)]$, expanding the product and regrouping the different terms, we obtain

$$\rho_L(q) = \frac{1}{q^{L-1}} \left[1 + \sum_{1\le i<j\le L} (q-1)^{j-i} B_{ij}\ + \sum_{1\le i<j<k<l\le L} (q-1)^{j-i+l-k}\ B^{(2)}_{i,j,k,l} + \cdots \right] \tag{10}$$

This gives the $\rho_L(q)$ in terms of the known $B_{i,j}$ and it can be used in this form. For example, for $L = 4$, it gives $\rho_4(q) = (8q^3 + 23q^2 + 12q + 1)/44q^3$ in agreement with what had been obtained by a direct calculation for small sizes [6].

An equivalent but more compact and manageable form can be obtained by defining two antisymmetric matrices $A_{ij} = -A_{ji} = -(q-1)^{j-i}$and $\mathrm{C_{ij}} = -\mathrm{C_{ji}} = \mathrm{B_{i,j}}$ for $1 \le \mathrm{i} < \mathrm{j} \le \mathrm{L}$. Eq.(10) can then be rewritten simply as [13],

$$\rho_L(q) = \frac{1}{q^{L-1}} \sqrt{\det(1 + \mathrm{AC})} \tag{11}$$

This expression (11) is our main exact result.

We have only been able to compute exactly the determinant of eq.(11) for q=0 (and 1!) [14]. For other values of q, we could only evaluate its asymptotic behavior. We summarize the main elements of our estimation which will be detailed elsewhere [14]. For large L, and i, j far from the boundaries, $B_{i,j}$ becomes a continuous function $\beta(x, y)$ of $x = i/L$ and $y = j/L$ which satisfies the Laplace equation (the continuous version of eq.(5)) with the boundary conditions $\beta(x, x) = 1,\ \beta(0, x) = \beta(x, 1) = 0$. This is a slowly varying function except in the two symmetric arbitrary small corners $0 \le x < y \ll 1$ and $1 - y < 1 - x \ll 1$ where its asympotic behavior is

$$\beta(x, y) = \beta(1 - y, 1 - x) = \frac{4}{\pi} \tan^{-1}(x/y), \quad \text{for } 0 < \mathrm{x} < \mathrm{y} \ll 1 \tag{12}$$

These two small neighbourhoods are responsible for the singular behavior of the determinant for large L. In the region $x < y \ll 1$, $\beta(x, y)$ is of the form $f(x/y)$ and the singular contribution can be obtained by computing the traces of the power of a Toeplitz matrix [15] in the variables $\log(x), \log(y)$. The same is true in the region $1 - y < 1 - x \ll 1$ where $\beta(x, y) \simeq f[(1-y)/(1-x)]$ (and with the variables $\log(1-x), \log(1-y)$). In this way we obtain for $1 \le q < 2$,

$$\theta(q) = -\int_{-\infty}^{\infty} \frac{dk}{4\pi}\ \log\left(1 - 2\frac{q-1}{q^2} \int_0^1 dx\ (x^{ik} + x^{-ik})\ f'(x)\right) \tag{13}$$

Using (12), this leads to (2) for $\theta(q)$. When $q > 2$, there is an additional term to (13) coming from an eigenvalue of the matrix $1 + AC$ which becomes very small as $L \to \infty$. As a consequence, (13) has to be replaced by its analytic continuation from the range $1 < q < 2$ and this leads again to (2).

In the whole range of q, the result (2) is in excellent agreement with previous numerical estimates [3,4,6]. For example, for $q = 5$, the exact prediction (2) gives $\theta(5) = .6928365..$ which agrees with the numerical estimate $.6928 \pm .0003$ of [6].

Our result (2) shows that systems as simple as the one dimensional Ising or Potts model at zero temperature exhibit rather complicated power law decays very similar to other irreversible processes such as reaction-diffusion [7,9] or sequential-parking [16] problems.

Result (2) is also reminiscent of the exactly known exponents [17] of the equilibrium Potts model in dimension 2. It would be interesting to see whether the methods originally used for these equilibrium problems or the more recent conformal theory techniques could be extended here to rederive (2).

We have already noted that expressions (7),(8),(10) and (11) are Pfaffians [12] which are always present in free fermion problems. In fact, another way of solving the coagulation model (with its boundary) consists in mapping it onto a free fermions problem. The details of this solution which requires several successive transformations of the original problem will be given in [14]. As the problem of the steady state of the reaction-diffusion is completely solved, one could calculate steady state properties such as density profiles, correlation functions. Also, as the whole problem can be reduced to a free fermion problem [14] (through unfortunately rather complicated transformations), one should be able to calculate all kinds of unequal time correlations.

Lastly, it is worth noting that the different scaling behaviors of $\rho_L(q)$ when q varies, arise in (2) from the asymptotic form of $P_L(m)$ for $L \gg 1$, $P_L(m) \sim \exp[\log L\, g(m/\log L)]$ where the function g is a Legendre transform of $2\theta(q)$ with respect to $\log(q)$ in a way quite reminiscent of the usual description of multifractal measures [18].

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[13] The reader can convince him/herself of the algebraic equivalence of eq.(10) and (11) by an explicit computation of the determinant for systems of small sizes ($L = 3, 4, ...$). The proof, which is not difficult, will be given in a longer and more detailed version of this work [14].
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